Welcome to STN International!   Enter x:x

LOGINID:SSSPTASXH1641

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * *   Welcome to STN International   * * * * * * * * * *

NEWS 1   Web Page URLs for STN Seminar Schedule - N. America
NEWS 2   "Ask CAS" for self-help around the clock
NEWS 3 SEP 09 ACD predicted properties enhanced in REGISTRY/ZREGISTRY
NEWS 4 OCT 03 MATHDI removed from STN
NEWS 5 OCT 04 CA/CAplus-Canadian Intellectual Property Office (CIPO) added
                 to core patent offices
NEWS 6 OCT 13 New CAS Information Use Policies Effective October 17, 2005
NEWS 7 OCT 17 STN(R) AnaVist(TM), Version 1.01, allows the export/download
                 of CAplus documents for use in third-party analysis and
                 visualization tools
NEWS 8 OCT 27 Free KWIC format extended in full-text databases
NEWS 9 OCT 27 DIOGENES content streamlined
NEWS 10 OCT 27 EPFULL enhanced with additional content
NEWS 11 NOV 14 CA/CAplus - Expanded coverage of German academic research
NEWS 12 NOV 30 REGISTRY/ZREGISTRY on STN(R) enhanced with experimental
                 spectral property data
NEWS 13 DEC 05 CASREACT(R) - Over 10 million reactions available
NEWS 14 DEC 14 2006 MeSH terms loaded in MEDLINE/LMEDLINE
NEWS 15 DEC 14 2006 MeSH terms loaded for MEDLINE file segment of TOXCENTER
NEWS 16 DEC 14 CA/CAplus to be enhanced with updated IPC codes
NEWS 17 DEC 16 MARPATprev will be removed from STN on December 31, 2005
NEWS 18 DEC 21 IPC search and display fields enhanced in CA/CAplus with the
                 IPC reform
NEWS 19 DEC 23 New IPC8 SEARCH, DISPLAY, and SELECT fields in USPATFULL/USPAT2

NEWS EXPRESS   JANUARY 03 CURRENT VERSION FOR WINDOWS IS V8.01,
               CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005.
               V8.0 USERS CAN OBTAIN THE UPGRADE TO V8.01 AT
               http://download.cas.org/express/v8.0-Discover/

NEWS DCOST   SINCE APPROXIMATELY 20:00 COLUMBUS TIME DECEMBER 29,
               SOME ONLINE COST DISPLAYS HAVE BEEN SHOWING COSTS IN
               2006 PRICES FOR STN COLUMBUS FILES. THIS HAS BEEN
               CORRECTED. PLEASE BE ASSURED THAT YOU WILL BE BILLED
               ACCORDING TO 2005 PRICES UNTIL JAN 1. PLEASE CONTACT
               YOUR LOCAL HELP DESK IF YOU HAVE ANY QUESTIONS. WE
               APOLOGIZE FOR THE ERROR.

NEWS HOURS   STN Operating Hours Plus Help Desk Availability
NEWS INTER   General Internet Information
NEWS LOGIN   Welcome Banner and News Items
NEWS PHONE   Direct Dial and Telecommunication Network Access to STN
NEWS WWW   CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
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* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 16:56:19 ON 04 JAN 2006

=>
Uploading
THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE
Do you want to switch to the Registry File?
Choice (Y/n):
Switching to the Registry File...
Some commands only work in certain files. For example, the EXPAND
command can only be used to look at the index in a file which has an
index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of
commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 16:56:31 ON 04 JAN 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file
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STRUCTURE FILE UPDATES: 3 JAN 2006   HIGHEST RN 871080-87-4
DICTIONARY FILE UPDATES: 3 JAN 2006   HIGHEST RN 871080-87-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

   Please note that search-term pricing does apply when
   conducting SmartSELECT searches.

****
*   *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005. A new display format, IDERL, is now   *
* available and contains the CA role and document type information. *
*   *
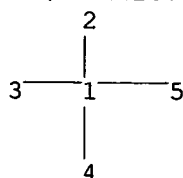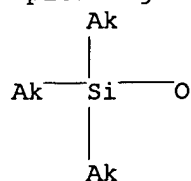***

Structure search iteration limits have been increased. See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

```
=>
Uploading C:\Program Files\Stnexp\Queries\10524207.str
      Ak                                              2
       |                                              |
       |                                              |
Ak——Si——O                              3———1———5
       |                                              |
       |                                              |
      Ak                                              4
```

```
chain nodes :
1   2   3   4   5
chain bonds :
1-2   1-3   1-4   1-5
exact/norm bonds :
1-2   1-3   1-4
exact bonds :
1-5
```

```
Match level :
1:CLASS   2:CLASS   3:CLASS   4:CLASS   5:CLASS
```

L1   STRUCTURE UPLOADED

```
=> d l1
L1 HAS NO ANSWERS
L1                    STR
      Ak
       |
       |
Ak——Si——O
       |
       |
      Ak
```
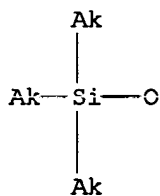
Structure attributes must be viewed using STN Express query preparation.

```
=> s l1
SAMPLE SEARCH INITIATED 16:56:45 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    24460 TO ITERATE

   8.2% PROCESSED     2000 ITERATIONS                           50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:   ONLINE   **COMPLETE**
                         BATCH    **COMPLETE**
PROJECTED ITERATIONS:        479844 TO    498556
PROJECTED ANSWERS:           315021 TO    330233

L2              50 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 16:56:53 FILE 'REGISTRY'
```

FULL SCREEN SEARCH COMPLETED -   487896 TO ITERATE

100.0% PROCESSED   487896 ITERATIONS   319576 ANSWERS
SEARCH TIME: 00.00.06

L3   319576 SEA SSS FUL L1

=> FIL CAPLUS
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                 ENTRY   SESSION
FULL ESTIMATED COST   166.94   167.15

FILE 'CAPLUS' ENTERED AT 16:57:05 ON 04 JAN 2006
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of this information, without the prior written consent of CAS, is
strictly prohibited.

FILE COVERS 1907 - 4 Jan 2006 VOL 144 ISS 2
FILE LAST UPDATED: 3 Jan 2006 (20060103/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l3
TOO MANY TERMS FOR FILE CROSSOVER IN L3
There are limits on the size of an answer set being crossed over from
one file to another. Enter HELP CROSSOVER at an arrow prompt (=>)
for specific information.

=> help crossover

 The term 'file crossover' refers to the use of an answer set L-number
 created by a search in one file as a search term or profile in
 another file. There are four types of crossovers in CAplus: query
 crossover, accession number crossover, crossover from the Registry
 File, and crossover of extracted terms.

 The query is searched in CAplus when you search the L-number answer
 set created in another file, except for CASREACT, MARPAT, MARPATprev,
 and Registry.

 Accession numbers are crossed over when you search an L-number answer
 set from CASREACT, MARPAT or MARPATprev in CAplus or when you search
 an L-number answer set from CAplus in MARPAT or MARPATprev.

 You may use the CAS Registry Numbers(R) that are answers from a
 search in the REGISTRY File as a search term or profile in the CAplus
 File, without looking at all the answers or entering the Registry
 Numbers individually. To do this, enter the L-number of the REGISTRY
 answer set in a SEARCH command in CAplus. You may use this L-number

in any search where you might use a Registry Number, i.e., combined
with other terms using the logical operators or the (L) operator.
Registry Numbers crossed over from the REGISTRY File include all
deleted (DR), replacing (RR), preferred (PR) and alternate (AR)
numbers.

CAS Registry Numbers appended by D or DP are automatically searched
whenever CAS Registry Numbers are crossed over. The suffix D
indicates a generic or unspecified derivative, and DP indicates the
preparation of generic derivatives. If you do not want to search CAS
Registry Numbers for nonspecific derivatives, append the crossover
L-number with /RN.

   Examples (where L3 is an answer set from the REGISTRY File):

      Search term   Retrieves

      => S L3   All CAS Registry numbers, including
                                  those appended with D or DP

      => S L3/RN   All CAS Registry Numbers,
                                  excluding those appended with D or DP

Additionally, the REGISTRY File answer set may be qualified by a code
for a CAS Role. Enter HELP ROLES at an arrow prompt (=>) in this
file to obtain a list of role codes and their definitions.

   Example of a search for Registry Numbers with the role code
   ANT for the role of "analyte" (where L3 is an answer set from the
   REGISTRY File):

      => S L3/ANT

There is a limit of 300,000 answers for a single crossover of CAS
Registry Numbers. For information on how to transfer more than
300,000 CAS Registry Numbers from the REGISTRY File, enter HELP
CROSSOVER at an arrow prompt in REGISTRY.

You may also crossover and search a set of terms extracted from an
answer set.

To crossover records from CAplus to CAOLD, use SELECT or TRANSFER
with the OREF field. The OREF (Original Reference Number) field
contains the Original Reference Number(s) for any record published in
printed CA in 1907-1966. The format of OREF is the volume number of
CA, colon, column number and fraction designation for the location of
the entire bibliographic record and the abstract on the page of
printed CA.

Enter HELP OREF for an example of a crossover from CAplus to CAOLD.
For more information on crossover of extracted terms, enter HELP
TRANSFER at an arrow prompt.

=> s l3/RN
TOO MANY TERMS FOR FILE CROSSOVER IN L3
There are limits on the size of an answer set being crossed over from
one file to another. Enter HELP CROSSOVER at an arrow prompt (=>)
for specific information.

=> s l3 and fluorine
TOO MANY TERMS FOR FILE CROSSOVER IN L3
There are limits on the size of an answer set being crossed over from

one file to another.   Enter HELP CROSSOVER at an arrow prompt (=>)
for specific information.

=> s 13/ant
TOO MANY TERMS FOR FILE CROSSOVER IN L3
There are limits on the size of an answer set being crossed over from
one file to another.   Enter HELP CROSSOVER at an arrow prompt (=>)
for specific information.

=> s 13/fluorine
TOO MANY TERMS FOR FILE CROSSOVER IN L3
There are limits on the size of an answer set being crossed over from
one file to another.   Enter HELP CROSSOVER at an arrow prompt (=>)
for specific information.

=> help crossover

 The term 'file crossover' refers to the use of an answer set L-number
 created by a search in one file as a search term or profile in
 another file.   There are four types of crossovers in CAplus: query
 crossover, accession number crossover, crossover from the Registry
 File, and crossover of extracted terms.

 The query is searched in CAplus when you search the L-number answer
 set created in another file, except for CASREACT, MARPAT, MARPATprev,
 and Registry.

 Accession numbers are crossed over when you search an L-number answer
 set from CASREACT, MARPAT or MARPATprev in CAplus or when you search
 an L-number answer set from CAplus in MARPAT or MARPATprev.

 You may use the CAS Registry Numbers(R) that are answers from a
 search in the REGISTRY File as a search term or profile in the CAplus
 File, without looking at all the answers or entering the Registry
 Numbers individually.   To do this, enter the L-number of the REGISTRY
 answer set in a SEARCH command in CAplus.   You may use this L-number
 in any search where you might use a Registry Number, i.e., combined
 with other terms using the logical operators or the (L) operator.
 Registry Numbers crossed over from the REGISTRY File include all
 deleted (DR), replacing (RR), preferred (PR) and alternate (AR)
 numbers.

 CAS Registry Numbers appended by D or DP are automatically searched
 whenever CAS Registry Numbers are crossed over.   The suffix D
 indicates a generic or unspecified derivative, and DP indicates the
 preparation of generic derivatives.   If you do not want to search CAS
 Registry Numbers for nonspecific derivatives, append the crossover
 L-number with /RN.

   Examples (where L3 is an answer set from the REGISTRY File):

     Search term   Retrieves

     => S L3   All CAS Registry numbers, including
                              those appended with D or DP

     => S L3/RN   All CAS Registry Numbers,
                              excluding those appended with D or DP

 Additionally, the REGISTRY File answer set may be qualified by a code
 for a CAS Role.   Enter HELP ROLES at an arrow prompt (=>) in this
 file to obtain a list of role codes and their definitions.

Example of a search for Registry Numbers with the role code
ANT for the role of "analyte" (where L3 is an answer set from the
REGISTRY File):

    => S L3/ANT

There is a limit of 300,000 answers for a single crossover of CAS
Registry Numbers. For information on how to transfer more than
300,000 CAS Registry Numbers from the REGISTRY File, enter HELP
CROSSOVER at an arrow prompt in REGISTRY.

You may also crossover and search a set of terms extracted from an
answer set.

To crossover records from CAplus to CAOLD, use SELECT or TRANSFER
with the OREF field. The OREF (Original Reference Number) field
contains the Original Reference Number(s) for any record published in
printed CA in 1907-1966. The format of OREF is the volume number of
CA, colon, column number and fraction designation for the location of
the entire bibliographic record and the abstract on the page of
printed CA.

Enter HELP OREF for an example of a crossover from CAplus to CAOLD.
For more information on crossover of extracted terms, enter HELP
TRANSFER at an arrow prompt.

=>
Uploading C:\Program Files\Stnexp\Queries\10524207a.str
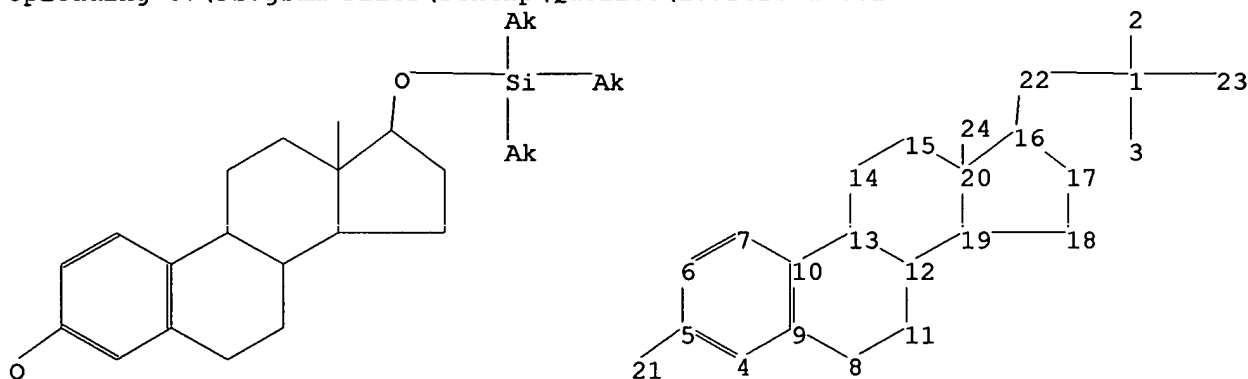
chain nodes :
1 2 3 21 22 23 24
ring nodes :
4   5   6   7   8   9   10   11   12   13   14   15   16   17   18   19   20
chain bonds :
1-2   1-3   1-22   1-23   5-21   16-22   20-24
ring bonds :
4-5   4-9   5-6   6-7   7-10   8-9   8-11   9-10   10-13   11-12   12-13   12-19   13-14   14-15
   15-20   16-17   16-20   17-18   18-19   19-20
exact/norm bonds :
1-2   1-3   1-23   5-21   16-22
exact bonds :
1-22   8-9   8-11   10-13   11-12   12-13   12-19   13-14   14-15   15-20   16-17   16-20
17-18   18-19   19-20   20-24
normalized bonds :
4-5   4-9   5-6   6-7   7-10   9-10
isolated ring systems :
containing 4 :

Match level :
1:CLASS 2:CLASS 3:CLASS 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:CLASS 22:CLASS 23:CLASS 24:CLASS

L4   STRUCTURE UPLOADED

=> FIL REGISTRY
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                          ENTRY   SESSION
FULL ESTIMATED COST   9.66   176.81

FILE 'REGISTRY' ENTERED AT 17:09:25 ON 04 JAN 2006
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STRUCTURE FILE UPDATES: 3 JAN 2006   HIGHEST RN 871080-87-4
DICTIONARY FILE UPDATES: 3 JAN 2006   HIGHEST RN 871080-87-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

   Please note that search-term pricing does apply when
   conducting SmartSELECT searches.

****
*   *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005. A new display format, IDERL, is now   *
* available and contains the CA role and document type information. *
*   *
****

Structure search iteration limits have been increased. See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> s l4
SAMPLE SEARCH INITIATED 17:09:31 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   67 TO ITERATE

100.0% PROCESSED   67 ITERATIONS   22 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH   **COMPLETE**

```
PROJECTED ITERATIONS:        849 TO      1831
PROJECTED ANSWERS:           159 TO       721


L5           22 SEA SSS SAM L4

=> s l5 sss full
FULL SEARCH INITIATED 17:09:45 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     1390 TO ITERATE

100.0% PROCESSED     1390 ITERATIONS                     518 ANSWERS
SEARCH TIME: 00.00.01


L6          518 SEA SSS FUL L4

=> FIL CAPLUS
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                ENTRY        SESSION
FULL ESTIMATED COST                            166.94        343.75

FILE 'CAPLUS' ENTERED AT 17:09:50 ON 04 JAN 2006
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FILE COVERS 1907 - 4 Jan 2006  VOL 144 ISS 2
FILE LAST UPDATED: 3 Jan 2006  (20060103/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l6
L7          165 L6

=> s l7 and (fluoride or fluorine)
        244734 FLUORIDE
         44140 FLUORIDES
        260172 FLUORIDE
               (FLUORIDE OR FLUORIDES)
         98401 FLUORINE
           521 FLUORINES
         98691 FLUORINE
               (FLUORINE OR FLUORINES)
L8            4 L7 AND (FLUORIDE OR FLUORINE)

=> d l8 ibib abs hitstr tot

L8    ANSWER 1 OF 4  CAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:        2004:1037341  CAPLUS
DOCUMENT NUMBER:         142:18635
TITLE:                   Determination of fluoride or hydrogen
```

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004104579	A1	20041202	WO 2004-FR50194	.20040514

```
        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
           CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
           GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
           LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
           NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
           TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
       RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
           AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
           EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
           SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
           SN, TD, TG
```

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
FR 2865540	A1	20050729	FR 2003-50160		20030520
FR 2865541	A1	20050729	FR 2003-50167		20030522
CA 2495558	AA	20041202	CA 2004-2495558		20040514
BR 2004006175	A	20050719	BR 2004-6175		20040514
US 2005227368	A1	20051013	US 2005-524207		20050210
PRIORITY APPLN. INFO.:			FR 2003-50160	A	20030520
			FR 2003-50167	A	20030522
			WO 2004-FR50194	W	20040514

```
OTHER SOURCE(S):           MARPAT 142:18635
```

AB The invention relates to a method for the detection and/or determination
    fluoride or HF in a sample. The sample is treated with a silylated
    organic compound in an aqueous solution in order to obtain a measuring
solution The organic
    silyl compound is desilylated by **fluoride** or HF, whereby the
    silylated organic compound and the deilsylated organic compound can be detected
    and/or dosed in a distinct manner. The appearance of the desilylated organic
    compound or the disappearance of the organic silylated compound which occurs if
    fluoride or hydrogen **fluoride** is present, is determined in
    the measuring solution The silylated organic compds. are estradiol, peptides,
    homovanillic acid, amphotericin, steroids, cytokines and arachidonic acid.
    The silylated organic compds. and the deilsylated organic compound can be
detected
    and determined by gas chromatog. or immunoassay. The invention makes it
    possible to detect in a very practical and easy manner the presence of HF
    or **fluoride** in concns. of 10-2 L of/ 106 L air (10 ppb), or even
    0.5-1 g/mL HF in a solution The inventive kit comprises the elements which
    are required to carry out said method. The inventive method makes it
    possible to detect **fluoride** in concns. of 0,001 g/mL.

```
IT  799775-62-5
    RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
        (reagent in determination of fluoride or hydrogen fluoride
        in environmental samples)
RN  799775-62-5  CAPLUS
CN  Acetic acid, [[(17β)-17-[(trimethylsilyl)oxy]estra-1,3,5(10)-trien-3-
    yl]oxy]- (9CI)  (CA INDEX NAME)


Absolute stereochemistry.
```

SiMe3
O

Me
S

S
S H S
H

R

H H

HO2C O
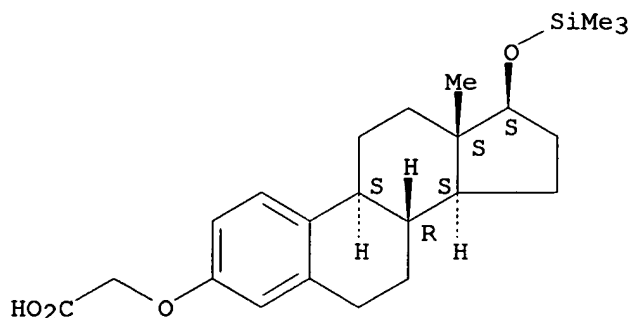
REFERENCE COUNT: 4   THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS
                                 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

AB   This report describes a concept in which an immunoassay is used indirectly
      to quantify a nonantigenic very low mol. weight compound participating in a
      chemical reaction with a haptenic reporter. The detection limit of each
      reagent is, therefore, governed only by the affinity of the antibodies
      toward the reporter. **Fluoride** was used as a model, and
      silylated estradiol was used as a reporter. Upon silylation with
      N-O-bis(trimethylsilyl)trifluoroacetamide (BSTFA) or N-O-
      bis(dimethylterbutylsilyl) trifluoroacetamide (MTBSTFA), estradiol is no
      longer recognized by antibodies specific to estradiol. After reaction
      with hydrofluoric acid (HF) or **fluoride** salts (KF, CsF, NaF),
      its immunoreactivity is restored, and native estradiol is formed and is
      detected by immunoassay. The level of synthesized estradiol is dependent
      on the concentration of **fluoride**. A **fluoride** detection limit
      of 0.3 μg/L (15 nM) is obtained. Potential interference with other
      acids has been eliminated by choosing the silyl group (trimethylsilyl vs.
      tert-butyldimethylsilyl) and by selecting optimal reaction conditions for
      the desilylation. The method has been applied to the detection of
      fluoride salts in natural waters (range 0.28-9.0 mg/L) and in an
      atmospheric artificially contaminated with HF between 8 and 160 μg/m3 in the
      parts-per-billion range. This indirect immunoassay combines simplicity
      and high sensitivity and, therefore, can be used in field monitoring.
      Finally, the extension of the concept to other chems. is discussed.
IT   **57711-41-8P 96013-91-1P**
      RL: ARU (Analytical role, unclassified); SPN (Synthetic preparation); ANST
      (Analytical study); PREP (Preparation)
         (detection of chems. by reporter immunoassay)
RN   57711-41-8   CAPLUS
CN   Silane, [[(17β)-estra-1,3,5(10)-triene-3,17-diyl]bis(oxy)]bis[(1,1-
      dimethylethyl)dimethyl- (9CI)   (CA INDEX NAME)
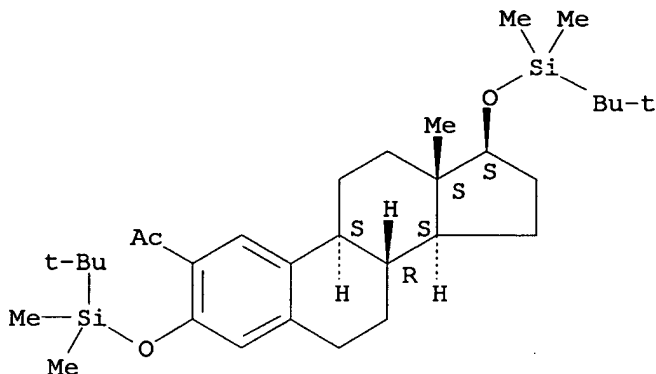
Absolute stereochemistry.
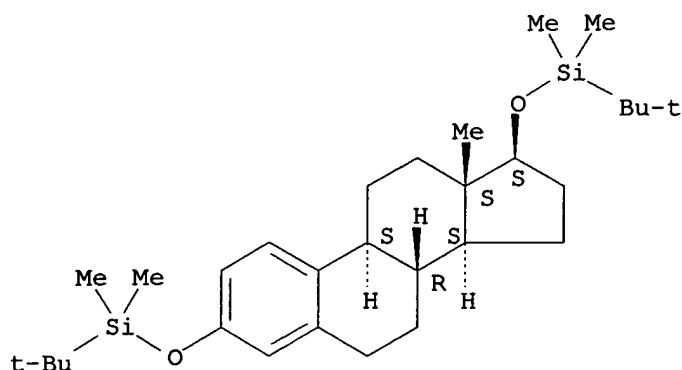
RN   96013-91-1 CAPLUS
CN   Estra-1,3,5(10)-trien-3-ol, 17-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-,
      (17β)- (9CI)   (CA INDEX NAME)

Absolute stereochemistry.
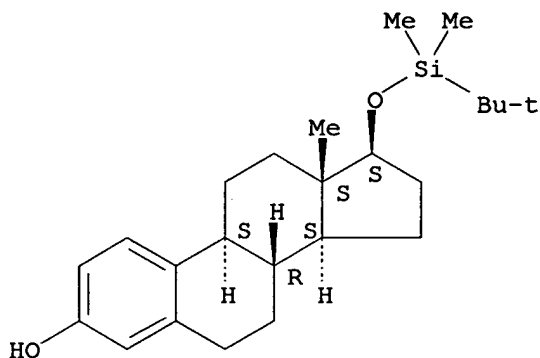
REFERENCE COUNT: 32   THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS
                                 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8   ANSWER 3 OF 4   CAPLUS   COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:751091   CAPLUS
DOCUMENT NUMBER: 124:30103
TITLE: A Novel 1,3 O → C Silyl Shift and Deacylation
                          Reaction Mediated by Tetra-n-butylammonium
                          Fluoride in an Aromatic System
AUTHOR(S):   He, Hu-Ming; Fanwick, Phillip E.; Wood, Karl; Cushman,
                          Mark
CORPORATE SOURCE: Department of Medicinal Chemistry and Pharmacognosy,
                          Purdue University, West Lafayette, IN, 47907, USA
SOURCE: Journal of Organic Chemistry (1995), 60(18), 5905-9
                          CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S):   CASREACT 124:30103
AB   A novel 1,3 O → C migration of a silyl group accompanied by a
      deacylation reaction was discovered during the conversion of
      2-acetyl-3,17-bis(tert-butyldimethylsilyl)-β-estradiol and
      3,17-bis(tert-butyldimethylsilyl)-2-propionyl-β-estradiol to
      2,17-bis(tert-butyldimethylsilyl)-β-estradiol in the presence of
      tetra-n-butylammonium fluoride. A crossover experiment indicated
      that the transformation is intramol.
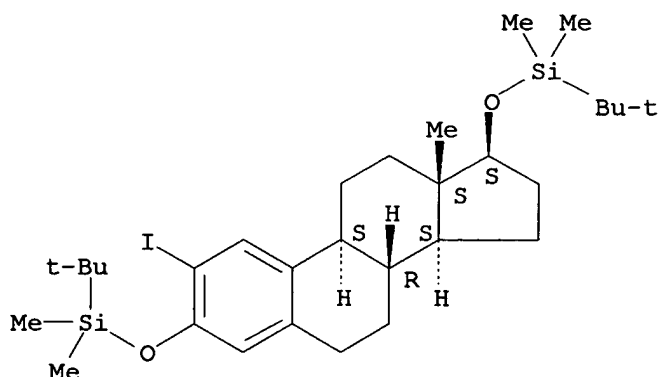
Absolute stereochemistry.

Absolute stereochemistry.

Absolute stereochemistry.
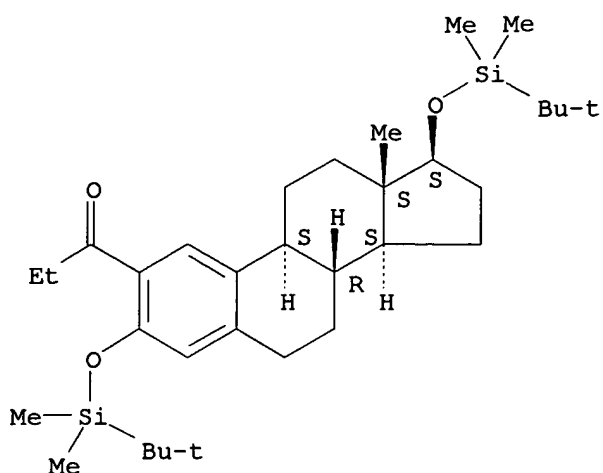
RN   168131-88-2 CAPLUS
CN   Estra-1,3,5(10)-trien-3-ol, 2-[(1,1-dimethylethyl)dimethylsilyl]-17-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN   168131-89-3 CAPLUS
CN   Estra-1,3,5(10)-trien-3-ol, 2-[(1,1-dimethylethyl)dimethylsilyl]-17-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-, acetate, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
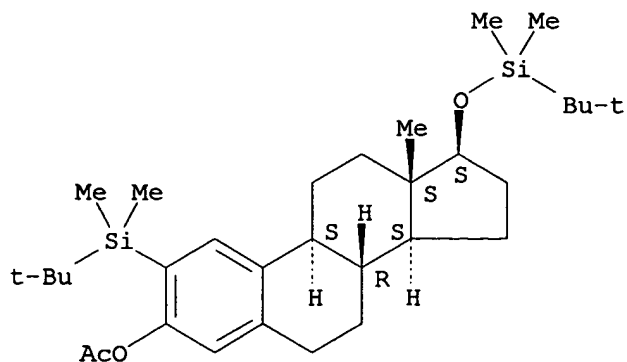
RN   168131-92-8 CAPLUS

Absolute stereochemistry.

Absolute stereochemistry.

Absolute stereochemistry.

AB   The selective deprotection of alc. or phenolic tert-butyldimethylsilyl
      ethers is described. The alc. ethers are deprotected with aqueous HF in MeCN,
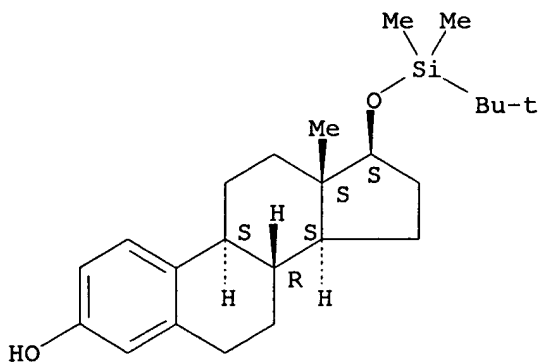   whereas phenolic ethers are deprotected with Bu4N+F- in THF.
IT   **96013-91-1P**
      RL: SPN (Synthetic preparation); PREP (Preparation)
          (preparation of)
RN   96013-91-1   CAPLUS
CN   Estra-1,3,5(10)-trien-3-ol, 17-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-,
      (17β)- (9CI)   (CA INDEX NAME)

Absolute stereochemistry.

IT   **57711-41-8**
      RL: PROC (Process)
          (selective deprotection of, with hydrogen **fluoride** or
          tetrabutylammonium **fluoride**)
RN   57711-41-8 CAPLUS
CN   Silane, [[(17β)-estra-1,3,5(10)-triene-3,17-diyl]bis(oxy)]bis[(1,1-
      dimethylethyl)dimethyl- (9CI)   (CA INDEX NAME)

Absolute stereochemistry.


```
=> FIL REGISTRY
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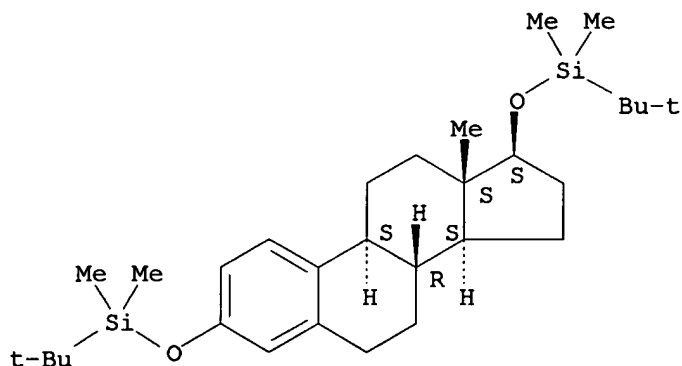
COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	28.02	371.77

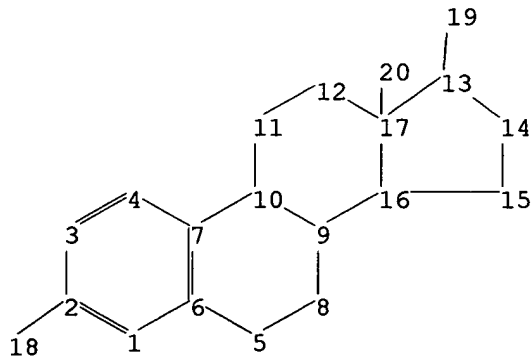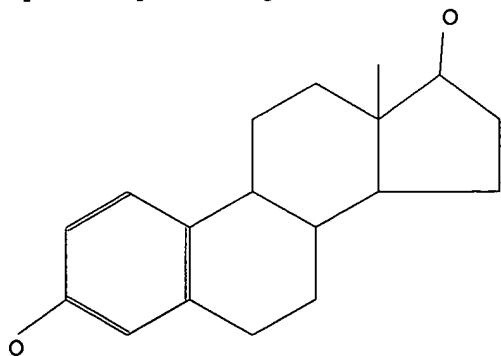| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-3.00	-3.00

Structure search iteration limits have been increased. See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10524207b.str

chain nodes :
18 19 20
ring nodes :
1   2   3   4   5   6   7   8   9   10 11 12 13 14 15 16 17
chain bonds :
2-18   13-19   17-20
ring bonds :
1-2 1-6 2-3 3-4 4-7 5-6 5-8 6-7 7-10 8-9 9-10 9-16 10-11 11-12 12-17
13-14 13-17 14-15 15-16 16-17
exact/norm bonds :
2-18   13-19
exact bonds :
5-6 5-8 7-10 8-9 9-10 9-16 10-11 11-12 12-17 13-14 13-17 14-15 15-16
16-17 17-20
normalized bonds :
1-2 1-6 2-3 3-4 4-7 6-7
isolated ring systems :
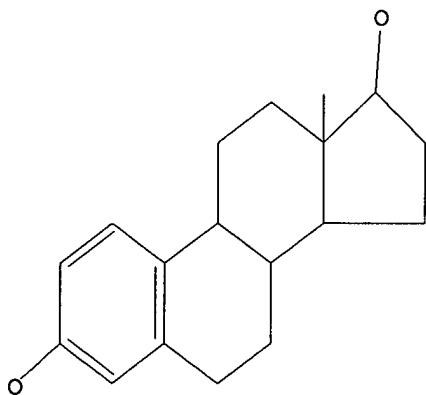containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS
20:CLASS

L9   STRUCTURE UPLOADED

=> d 19
L9 HAS NO ANSWERS
L9   STR

Structure attributes must be viewed using STN Express query preparation.

=> s 19
SAMPLE SEARCH INITIATED 17:15:17 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   1646 TO ITERATE

100.0% PROCESSED   1646 ITERATIONS   50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE   **COMPLETE**
                         BATCH   **COMPLETE**
PROJECTED ITERATIONS: 30487 TO   35353
PROJECTED ANSWERS: 13017 TO   16263

L10   50 SEA SSS SAM L9

=> s 19 sss full
FULL SEARCH INITIATED 17:15:25 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   32777 TO ITERATE

100.0% PROCESSED   32777 ITERATIONS   14455 ANSWERS
SEARCH TIME: 00.00.01

L11   14455 SEA SSS FUL L9

=> FIL CAPLUS
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                 ENTRY   SESSION
FULL ESTIMATED COST   166.94   538.71

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)   SINCE FILE   TOTAL
                                                 ENTRY   SESSION
CA SUBSCRIBER PRICE   0.00   -3.00

FILE 'CAPLUS' ENTERED AT 17:15:30 ON 04 JAN 2006
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FILE COVERS 1907 - 4 Jan 2006   VOL 144 ISS 2
FILE LAST UPDATED: 3 Jan 2006   (20060103/ED)

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=> s l11
L12   75208 L11

=> s l12 and (fluoride or fluorine)
       244734 FLUORIDE
        44140 FLUORIDES
       260172 FLUORIDE
               (FLUORIDE OR FLUORIDES)
        98401 FLUORINE
          521 FLUORINES
        98691 FLUORINE
               (FLUORINE OR FLUORINES)
L13   232 L12 AND (FLUORIDE OR FLUORINE)

=> s l13 and (detect? or measur?)
      1528769 DETECT?
      2816615 MEASUR?
L14   45 L13 AND (DETECT? OR MEASUR?)

=> s l14 and (silicon or silica or silylat?)
       750020 SILICON
          445 SILICONS
       750180 SILICON
               (SILICON OR SILICONS)
       487203 SILICA
         3723 SILICAS
       487613 SILICA
               (SILICA OR SILICAS)
        25297 SILYLAT?
L15   3 L14 AND (SILICON OR SILICA OR SILYLAT?)

=> s l15 not l8
L16   1 L15 NOT L8

=> d 116 ibib abs hitstr tot

L16 ANSWER 1 OF 1 CAPLUS   COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1983:83043 CAPLUS
DOCUMENT NUMBER: 98:83043
TITLE: Boron trifluoride etherate as a spray reagent for the
                         detection of steroids and triterpenoids by TLC
AUTHOR(S):   Ghosh, Parthasarathi; Thakur, Swapnadip
CORPORATE SOURCE: Dep. Chem., Univ. Burdwan, Burdwan, 713104, India
SOURCE: Fresenius' Zeitschrift fuer Analytische Chemie (1982),
                         313(2), 144
                         CODEN: ZACFAU; ISSN: 0016-1152
DOCUMENT TYPE: Journal
LANGUAGE: English

B trifluoride etherate was used as a spray reagent for the
detection of steroids and triterpenoids on **silica** gel-G
thin-layer chromatog. (TLC) plates. After developing with 1:1
benzene-EtOAc, the plates were sprayed with the reagent and heated for 5
min at 125° to produce colored spots. The color reactions and
detection limits are given for some steroids and triterpenoids.

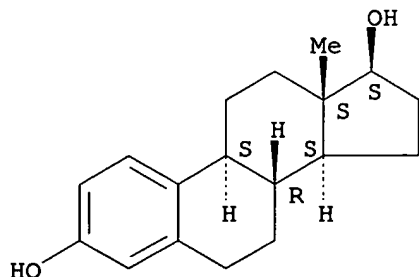IT   **50-28-2,** analysis **57-63-6 72-33-3**
     RL: ANT (Analyte); ANST (Analytical study)
       (**detection** of, boron trifluoride etherate in thin-layer
       chromatog.)

RN   50-28-2 CAPLUS
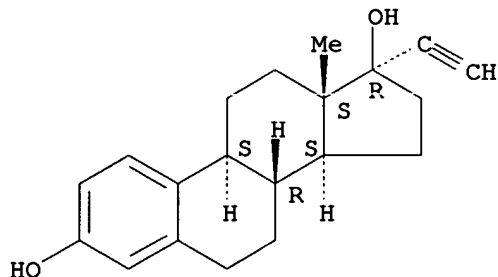CN   Estra-1,3,5(10)-triene-3,17-diol (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN   57-63-6 CAPLUS
CN   19-Norpregna-1,3,5(10)-trien-20-yne-3,17-diol, (17α)- (9CI) (CA
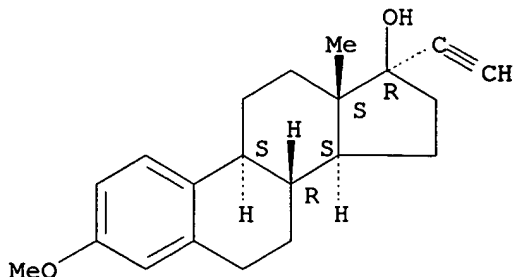   INDEX NAME)

Absolute stereochemistry.

RN   72-33-3 CAPLUS
CN   19-Norpregna-1,3,5(10)-trien-20-yn-17-ol, 3-methoxy-, (17α)- (9CI)
     (CA INDEX NAME)

Absolute stereochemistry.

```
=> s 114 and hydrofluoric acid
        23005 HYDROFLUORIC
      4081719 ACID
      1505424 ACIDS
      4567282 ACID
                (ACID OR ACIDS)
        22560 HYDROFLUORIC ACID
                (HYDROFLUORIC(W)ACID)
L17           1 L14 AND HYDROFLUORIC ACID

=> s 117 not 18
L18           0 L17 NOT L8

=> s 114 and fluorine
        98401 FLUORINE
          521 FLUORINES
        98691 FLUORINE
                (FLUORINE OR FLUORINES)
L19          22 L14 AND FLUORINE

=> s 119 and silyla?
        29955 SILYLA?
L20           0 L19 AND SILYLA?

=> log y
```

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	33.46	572.17

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.75	-3.75

STN INTERNATIONAL LOGOFF AT 17:24:16 ON 04 JAN 2006